The density of the crystal measured by floatation method was 1.41 gm/cc and that calculated with 2 molecules per unit cell was 1.423 gms/cc.

Evidences from the morphology of the crystal, intensity, statistics (Howells *et al* 1950) as well as the number of molecules per unit cell suggest the space group to be P $\bar{1}$. Pyroelectric tests on the crystal gave negative results.

A full investigation of the crystal structure using Fourier techniques and partial thee-dimensional data is in progress, the details of which will be published later.

The authors wish to acknowledge with thanks the gift of the sample of homopathalic acid by Dr J. N. Chatterjee of the chemical laboratories, Science College, Patna. One of us (S. B.) is indebted to the University Grants Commission of India, New Delhi, for the award of a Junior Fellowship during the tenure of which this work is being pursued. The authors also thank Prof. K. Lonsdale, F. R. S. of the University College, London in whose laboratory pyroelectric tests on the crystal were carried out.

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On the co-efficient of molecular packing in some dicarboxylic acids.

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(Received 20 February 1967)

Kitaigorodski (1961) has put forward the theory that "a crystal of an organic compound can be considered as a system of closely packed layers, the molecules within a layer are also very closely packed, having co-ordination numbers of six and being so arranged that no polarities appear perpendicular to the layer". He has also suggested that "the intermolecular radii elements found in organic compounds are universal and reasonably constant *i. e.* applicable to all molecules. They can be used to assign definite shapes to molecules. If, after the molecules have been built up from intermolecular radii, we consider the molecular posi-

tioning found by expeiment, it appears that all the molecules are in contact none are suspended in empty space and none interpenetrate". According to this view, the crystal structures of organic molecules were governed solely by the close-packing principles and one could predict the organic crystal structures in the various space groups by regarding the molecules in them as being built up from the close packing of atoms with rigid spherical shapes, where rigid spherical contact radii could be specified to within 0.1 Å. Kitaigorodskii defines a quantity $K = Z\frac{V_o}{V}$ which he calls the packing density "co-efficient of molecular packing", where Z = number of the molecules in the cell, V_o = molecular volume calculated from the contacts of rigid sphere (truncated for chemical bonding, where necessary), V = volume of the unit cell.

The value of 'K' ranges from 0.68 to 0.887 (Graphite) whereas the theoretical value for closed-packed spheres is 0.74. K increases from values below 0.70 to theoretical value of 0.74 for closed packed spheres as the molecular shape tends to become more spherical or ellipsoidal.

In course of testing Kitaigordskii's theory, the authors have calculated (table 1) the coefficients of molecular packing in some simple dicarboxylic acids whose crystal structures are well known or have been established very recently by X-ray Fourier analysis. In calculating these coefficients, Kitaigorodskii's empirical rule has been followed than "while calculating volumes and constructing models, the H-atoms participating in hydrogen bonds should be neglected, while the X-atoms to which they are valence-bonded should be taken as spherical in the X-H direction."

TABLE 1 INTERMOLECULAR RADII C=1.90 Å, O=1.35 Å

Molecule	Molecular volume V (A^{3a})	Molecular packing co-efficient K	Reference
α-oxalic acid	57.73	0.751	Cox *et al* (1952)
β-oxalic acid	57.73	0.731	Hendricks (1935)
Oxalic acid dihydrate	57.73	0.618	Ahmed and Cruickshank (195
Acetylene dicarboxylic acid dihydrate	113.17	0.671	Robertson (1947)
Dihydroxyfumaric acid dihydrate	111.0	0.620	Gupta (1964)

However, if one assumes a value for the intermolecular radius as actually found in the crystal structure (*e. g.* determined from the shortest carbon-carbon or carbon-oxygen contact distances), the values for the coefficient of molecular packing changes significantly as may be seen from comparison of table 1 and table 2 (given below).

TABLE 2

Molecule	Molecular volume V_0 (Å)	K Molecular packing coefficient	Shortest distances calculated Å	Assumed value of intermolecular radius	
				C (Å)	O (Å)
α-oxalic acid	63.40	0.811	C—C 3.93 C—O 3.37	1.97	1.40
β-oxalic acid	56.19	0 700	C—C 3.71 C—O 3.35	1.86	1.49
oxalic acid dihydrate	71 07	0.556	C—C 3.60 C—O 3 16	1.80	1.36
Acetylene dicarboxylic acid dihydrate	116.9	0.693	C—C 3.86 C—O 3.29	1.93	1.36
Dihydroxyfumaric acid dihydrate	118.87	0.664	C—C 3 97 C—O 3.40	1.98	1.42

As tables 1 and 2 above show, the values of intermolecular radii for the atoms are not universal constants as Kitaigorodskii claims but vary somewhat from crystal structure to crystal structure. This is admitted even by Kitaigorodskii (ibid) to be due to second order effects depending on relative orientation of the contact with respect to the chemical bonds near it (steric hindrances) and on the anisotropy of thermal vibrations.

It would, therefore, appear that packing consideration is not the only criterion determing the crystal structure of organic molecules as Kitaigorodskii suggests but secondary effects also play in important role.

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